

We claim:

1. A method which comprises
providing a PDF trace of a first sample of a substance,
providing a PDF trace of a second sample of the substance, and
comparing the PDF traces to determine whether the substance of the first sample and the substance of the second sample have the same or different solid forms.
2. A method as claimed in claim 1, wherein the substance is a chemical compound.
3. A method as claimed in claim 2, wherein the substance is a pharmaceutical compound.
4. A method as claimed in claim 3, wherein the pharmaceutical compound is a pharmaceutically acceptable salt.
5. A method as claimed in claim 1, wherein the substance is a mixture of two or more chemical compounds.
6. A method as claimed in claim 5, wherein the substance is a cocrystal.
7. A method as claimed in claim 5, wherein a compound in the mixture is water and the substance is a hydrate.
8. A method as claimed in claim 1, wherein the substance of at least one sample is disordered crystalline, and which comprises comparing the PDF traces to determine whether the substance of the first sample and the substance of the second sample have the same solid form, being related through disorder.
9. A method as claimed in claim 1, wherein the solid form of the substance of the first or second sample is a known solid form of the substance.

10. A method as claimed in claim 1, wherein at least one of the PDF traces is calculated based on a composite X-ray powder diffraction pattern derived from two or more measured X-ray powder diffraction patterns of the sample.

11. A method of screening for new solid forms of a substance, which comprises

providing a PDF trace of each of a plurality of test samples of a substance,
providing one or more PDF traces of known solid forms of the substance,
comparing the PDF traces of one or more of the test samples to one or more of the PDF traces of known solid forms to identify any substances in the test samples that have a new solid form.

12. A method which comprises

providing a PDF trace of each of a plurality of test samples of a substance,
and

grouping the plurality of PDF traces of the substance by similarity into two or more groups through hierarchical cluster analysis.

13. A system which comprises

means for providing a PDF trace of a first sample of a substance,
means for providing a PDF trace of a second sample of the substance, and
means for comparing the PDF traces to determine whether the substance of the first sample and the substance of the second sample have the same or different solid forms.

14. A computer-readable medium comprising instructions for performing the method as claimed in claim 1.